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A quantum chemical study of an interaction between collagen fragments and calcium ions using calculations of model complexes

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Abstract

© 2015 Springer Science+Business Media New York. Quantum chemical calculations revealed that the complexation between proline-containing collagen fragments and calcium ions involves a preferential interaction between Ca^{2+} ions and the oxygen and nitrogen atoms of proline in the glycine - proline - alanine fragment of the amino acid sequence of collagen.

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Keywords

amino acids, calcium ions, collagen fragments, density functional theory, gauge invariant atomic orbitals, natural bond orbitals, NMR shielding constants, the functional B3LYP